Charge Inhomogeneity in Correlated Electron Systems

<u>Description</u>: This program coordinates a multidisciplinary experimental and theoretical investigation of synthetic metals and doped insulators. The goal of this work is to search for experimental signatures of self-organized structures over a wide range of energy and length scales. A particular emphasis of the program is the coherent approach centered around a variety of experimental techniques, and a close collaboration with theory. Recent work has focused on the transition metal oxides, in particular, manganites, cuprates, nickelates, ruthenates, and cobaltates, both in bulk and thin film form.

Program Highlights

- Studied nanoscale structural correlations present in the insulating phase of the manganites. These appear to play a central role in the colossal magnetoresistance effect.
- Derived a coherent description of the low energy electronic properties of Sr₂RuO₄.
- Studied the thermodynamics related to the interplay of magnetism and superconductivity.
- Carried out inelastic xray scattering studies of insulating and doped cuprates, measuring the dispersion of the gap excitons for the first time with this technique.

<u>Impact</u>: This program has played a significant role in drawing together a number of different efforts within Condensed Matter Physics at BNL, stimulating new collaborations. Especially important has been the creation of an internal seminar series generally dedicated to correlated electron systems (see below).

<u>Interactions</u>: This program makes close connection between the groups within Condensed Matter Physics and with other departments at BNL, in particular, the NSLS and the Materials Science Department. Further, there are extensive external collaborators. Particularly important ones include: UCLA, U. Rutgers, U. Delaware, U. Toronto, U. Tokyo, Tohoku U., and HASYLAB.

<u>Personnel</u>: John M. Tranquada (10% Neutron Scattering), Victor Emery (50% Theory), Young-June Kim (70%, Research Associate in X-ray Scattering), Ralph Werner (85%, Research Associate in Theory), Christie Nelson (70% Research Associate in X-ray Scattering).

Recognition: Buckley Prize (Victor Emery, 2001), Goldhaber Fellowship (Young-June Kim, 2001).

Budget: \$240 K.

Scientific Staff

John M. Tranquada Superconductivity, antiferromagnetism, charge order in complex

oxides.

Victor Emery Strongly correlated electron systems, low-dimensional magnetism, and

statistical mechanics.

Young-June Kim Electronic excitations in 2D cuprates, xray and neutron scattering

studies of transition metal oxides.

Christie Nelson Orbital and charge ordering in transition metal oxides, including thin

films in particular, as studied with x-rays.

Ralph Werner Theory of strongly correlated electron systems and magnetism.

Future Directions

• A potentially highly exciting area that this effort may evolve towards is the study of nanostructural strongly correlated systems. Examples include nanopatterning of dopants in transition metal oxides and studies of confinement phenomena-which are expected to be quite different from those exhibited by simple (e.g., metallic or semiconductor) systems. This work forms one of the major thrust areas of the proposed BNL Nanocenter.

<u>Interactions</u>: One of the main goals of this program has been to strengthen the cross-connections between the various experimental and theoretical groups within condensed matter physics, and elsewhere in BNL. One mechanism for encouraging such interactions has been a series of informal seminars. Below are the speakers and titles of the first two years of the series:

Condensed matter informal seminars Correlated electron systems

Low temperature electronic properties of Sr₂RuO₄ Ralph Werner, Brookhaven National Laboratory (BNL)

Epitaxial ferroelectric heterostructures: writing electronic nanofeatures and electrostatic modulation of high T_c superconductivity

Charles Ahn, Yale University

Optical studies of charge dynamics in c-axis oriented superconducting MgB_2 films Jiufeng Tu, BNL

Theoretical perspectives on La_{1.5}Sr_{0.5}CoO₄ Oron Zachar, BNL

Scattering rate sum rule Christopher Homes, BNL

Infrared spectroscopy of high-T_c superconductors: new results Dimitri Basov, University of California at San Diego

Latest on MgB₂

BNL Staff (3 separate seminars, each with three speakers, on subject)

Line shapes in frustrated Heisenberg chains Ralph Werner, BNL

ARPES results from highly overdoped ($T_c \sim 51 K$) Bi2212 Zikri Yusof, BNL/University of Connecticut

Experimental evidence of spin-charge coupling in the optical studies of optimally doped Bi2212 and a metallic cobaltate
Jiufeng Tu, BNL

How to publish a paper in nature Leslie Sage, Editor of Nature, Washington, D.C.

Spin quantum hall transition: localization and percolation inside a superconductor Ilya Gruzberg, University of California

Antiferromagnetism and Fermi surface in Sr₂RuO₄ Ralph Werner, BNL

Correlated polarons in the paramagnetic insulating phase of dissimilar perovskite manganites Christie Nelson, BNL

Electrochemical mediated thin film growth Stanko Brankovic, BNL

On the glassy state of stripes in doped antiferromagnets Oron Zachar, International Center for Theoretical Physics, Trieste, Italy

Structural phase transitions and magnetism in La_2CuaO_4 isostructures Ralph Werner, BNL

Lattice modulation and metal insulator transition in La_{1-x}Sr_xMnO₃ thin films Assunta Vigliante, Max-Planck Institut Fur Metallforschung, Stuttgart, Germany

 $La_{2-x}M_xCuO_4$: structure in relationship with superconductivity, magnetism, and stripes Arnold Moodenbaugh, BNL

Field induced long range order and spin freezing in a Haldane-gap system Andrey Zheludev, ${\tt BNL}$

Correlated versus uncorrelated stripe pinning: the different roles of Nd and Zn co-doping C. Morais Smith, Univ. de Fribourg, Switzerland & Univ. Hamburg, Germany

Diagonal incommensurate spin density wave in lightly hole-doped $La_{2-y}Nd_ysr_xCuO_4$ Shuichi Wakimoto, BNL/MIT

The magnetic resonance and photoemission in cuprate superconductors Tony Valla & John Tranquada, BNL

Single-particle and continuum states in weakly-coupled s=1/2 quantum spin chains Andrey Zheludev, BNL

The ab-plane transport in Bi-2212: is there evidence for a superconducting gap? Tom Timusk, McMaster University, Hamilton, Ontario, Canada

Single-mode to continuum crossover in the Haldane spin chain Igor Zaliznyak, BNL

Understanding high and ultra-high piezoelectric response in perovskites Beatriz Noheda, BNL

Exotic superconductivity by conventional mechanisms Victor Barzykin, National High Magnetic Field Laboratory, Tallahassee, Florida

Correlated electrons in the borides and in transition metal alloys Richard Watson, BNL

 $\label{lem:macroscopic} \mbox{Macroscopic phase separation-chemical facts and physical fiction} \\ \mbox{Tom Vogt, BNL}$

Unidentified orbital ordering and secret Fermi surface maps in the rare earth polychalcogenides RX_n Elaine DiMasi, BNL

ARPES studies of Sr₂RuO₄: Fermi surface, excitation gaps, and dimensional crossover Alexei Fedorov, BNL

Optical properties of La₂NiO_{4.133} Christopher Homes, BNL

Charge and orbital order in transition metal oxides John P. Hill, BNL

Recent Research Highlights

Structural Correlations in Colossal Magnetoresistance Manganites

[Nelson, Hill, Gibbs (BNL), Kiryukhin, Cheong (Rutgers), Y. Tokura (U. Tokyo)]

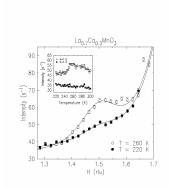


Fig. 1 Stuctural correlations in La_{0.7}Ca_{0.3}MnO₃ above (open circles) and below (closed circles) the Curie temperature. Inset shows the intensity of these correlations as a function of temperature.

Perovskite manganites have recently attracted renewed attention, both as examples of strongly correlated electron systems and because they exhibit so-called colossal magnetoresistance (CMR). At the heart of the CMR effect lies a magnetic field-driven metal-insulator transition. In a series of experiments, we have studied the paramagnetic insulating (PI) phase in a number of manganites. We find similar structural correlations (fig. 1) with both the same wave-vector and the same correlation length in three different manganites (Pr_{0.7}Ca_{0.3}MnO₃, La_{0.7}Ca_{0.3}MnO₃, and Nd_{0.7}Sr_{0.3}MnO₃) despite the fact that these exhibit quite different low temperature ground states. Further, experiments in an applied field suggest that these same correlations play an intimate role in the CMR effect. In particular, they disappear in the fieldinduced metallic phase unlike the scattering arising from uncorrelated distortions. Studies of the doping dependence reveal that the wavevector varies linearly with x for 0.3<x<0.5 in Nd_{1-x}Sr_xMnO₃. This work sheds new light on the mechanism of the CMR effect and the role of structural correlations.

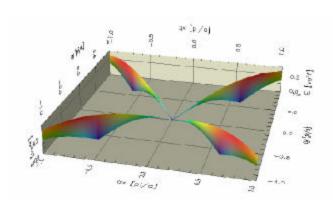
Refs: C.S. Nelson et al., PRB **64** 174405 (2001), V. Kiryukhin et al., PRB, Rapid Comm, (in press), V. Kiryukhin et al PRL (submitted).

Coherent description of the low energy electronic properties of Sr_2RuO_4 [R. Werner (BNL)]

Starting from the quasi-one-dimensional kinetic energy of the d_{yz} and d_{zx} bands we derive a bosonized description of the correlated electron system in Sr_2RuO_4 . At intermediate coupling the magnetic correlations are quasi one-dimensional and account for the observed neutron scattering results. Together with two-dimensional correlations accessible via perturbative approaches the normal phase specific heat, cyclotron mass enhancement, static susceptibility, and Wilson ratio are described consistently.

The body centered tetragonal structure of Sr_2RuO_4 gives rise to enhanced inter-plane pair correlations in the d_{yz} and d_{zx} orbitals. Using a bosonized description of the in-plane electron correlations the superconducting order parameter is found to be a mixed orbital spin-one doublet with two spatial components. The spatial anisotropy is 5%. The different components of the order parameter give rise to two-dimensional gapless fluctuations. The temperature dependence of the pair density, specific heat, NQR, Knight shift, and susceptibility are obtained, and found to be consistent with experiment.

Figure 2 shows the excitation spectrum of the quasi one-dimensional magnetic correlations. These contribute about 15% of the total normal phase linear specific heat coefficient and about 20% to the total uniform static susceptibility. The resulting magnetic structure factor has a finite q width even at zero temperature, in agreement with experiment [Y. Sidis *et al.* Phys. Rev. Lett. **83**, 1999].



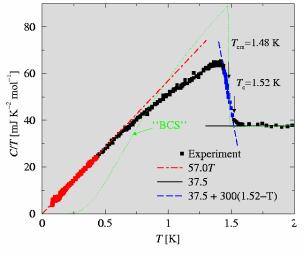


Figure 3 shows the specific heat divided by temperature, as a function of temperature through the superconducting transition. Symbols are from experiment [S. NishiZaki, Y. Maeno, and Z. Mao, J. Phys. Soc. Jpn. **69**, 572 (2000)]. $T_{\rm cm}$ =1.48 K is the "mid-transition" value. The actual transition is at $T_{\rm C}$ =1.52 K. In the normal phase, the specific heat is linear (full line). For T just below $T_{\rm C}$ a linear increase with t=1-T/ $T_{\rm C}$ (blue broken line) is observed while for T<0.3 K the specific heat is quadratic in temperature (dot-dashed red line), consistent with two-dimensional, gapless order parameter fluctuations. Dotted green line: sketch of the BCS contribution.

Thermodynamics of the Interplay between Magnetism and High-temperature Superconductivity [Emery (BNL), Kivelson (UCLA), Aeppli (NEC); cond-mat/0105200]

The phase diagrams of conventional superconductors are usually simple, with no ordered phases competing with the superconducting state. By contrast, the high temperature superconductors have a number of competing phases which appear as the temperature is lowered. One of the most astonishing manifestations of this competition occurs in the LaCuO family of materials where magnetism and high temperature superconductivity coexist.

The interplay between "stripe" magnetism and superconductivity can be understood most simply by treating the liquids of mobile charge carriers in the high-temperature superconductors as fluids with a variety of ground states. As for other complex fluids, the coupling between the order parameters can lead to phases with mesoscopic density modulations, as well as diverse combinations of the order parameters themselves. In the present case, the two coupled order parameters entering the Landau free energy are a vector representing the long period antiferromagnet and a complex parameter representing the superconducting order.

There are several generic phase diagrams derivable from such a Landau free energy, differing in the types of critical points. In Fig. 4a, phases with either magnetic or superconducting order exist, as well as a homogeneous intermediate phase with bulk coexistence of the two. In Fig. 4b, there is no bulk coexistence, but a region of two-phase coexistence of a hole-poor, magnetically ordered and a hole-rich, superconducting region. Because of the long-range Coulomb interaction between holes, macroscopic phase separation is thermodynamically forbidden, leading to a state which is inhomogeneous on an intermediate length scale. For a tricritical point (Fig. 4c), superconductivity (if it appears at all) manifests itself below a phase-boundary, and in Fig. 4d, phase separation occurs into hole-rich and hole-poor phases, neither of which is ordered.

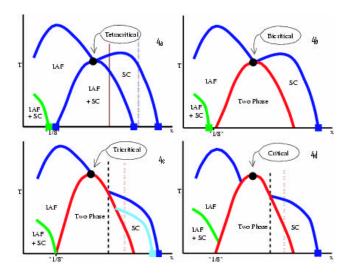


Fig. 4. Schematic phase diagrams derived from the Landau free energy. "IAF" and "SC" indicate incommensurate (striped) antiferromagnetic and superconducting order, respectively. Circles represent classical critical or multicritical points and the squares quantum critical points. The various vertical lines represent trajectories through the phase diagram. The pale blue phase boundary in c) represents the effect of an applied magnetic field on the phase diagram.

The thermal evolution of a given material should be associated with a trajectory in one of the generic phase diagrams; La_2CuO_{4+d} is associated with the vertical dashed line in Fig. 4c or 4d. It is special in the sense that it is tuned (by only one parameter) to pass close to the critical end point. Below T_c , the system forms an inhomogeneous mixture of a high-density superconducting and a low-density antiferromagnetic phase. At Tc, the sample is a single-phase superconductor, with a superconducting volume fraction that shrinks at the expense of the antiferromagnet as the temperature is reduced through the two-phase region. The growth of the magnetism is associated more with the growth of the hole-poor fraction than with the rise of the order parameter within the hole-poor regions.

Not only is this scenario consistent with the simultaneous onset of superconductivity and magnetism, it also reconciles the neutron scattering and μ -SR data. A miscibility gap in the phase diagram not only resolves old puzzles, but also provides a framework for understanding current and future experiments. Particularly important are measurements of magnetic field-dependent effects, as they permit a continuous variation of the parameters in the Landau free energy, as seen in Fig. 4c.

<u>Publications</u>: Below is a list of publications in which one or more of the co-authors were funded by this program. These papers are also included in the respective group publication lists as denoted by $\mathbf{X}(=\mathbf{X}-\mathbf{ray})$, $\mathbf{N}(=\mathbf{Neutron Scattering})$, $\mathbf{E}(=\mathbf{Electron Spectroscopy})$, $\mathbf{P}(=\mathbf{Powder Diffraction})$, and $\mathbf{T}(=\mathbf{Theory})$.

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